ISBN: 978-3-95450-184-7 doi:10.18429/JACoW-IPAC2018-THPMF084

NUMERICAL SHOT NOISE MODELING AND PARTICLE MIGRATION SCHEME*

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Abstract

In order to model correct statistical properties of shot noise, special particle loading algorithms were developed and used in FEL community. However, the compatibility of such loading algorithms with particle migration scheme across numerical mesh is not well studied. Here, we address the necessity of special particle migration scheme for different loading algorithms and present a possible solution.

INTRODUCTION

The memory efficient FEL codes like GENESIS [1] used to simulate the electron bunch from the tail to the head sequentially keeping only one temporal slice of the bunch in memory. This restricts particle migration across the temporal mesh of numerical discretization. Such restriction prevents reliable modeling of the evolution of temporal electron bunch profile. On the other hand, in order to reduce numerical shot noise, special particle loading methods are used in FEL codes. Therefore, care must be taken when particle migration is implemented. An intuitive solution would be to keep the whole bunch in memory and simulate it through lattice while allowing individual particles to migrate. However, as will be shown later, such a straightforward solution can produce the numerical shot noise much larger than the physical shot-noise depending on the used particle loading method. In this paper, we discuss a solution pair, i.e. a particle loading and corresponding discretization scheme, to the particle migration problem.

REVIEW OF SHOT NOISE MODELING METHODS

In order to build a method for particle migration, we need a good physical interpretation of each particle for a given particle loading method. In this section, we review two widely used particle loading methods.

Charge Perturbation and Volume Division

McNeil et al. [2] proposed a shot-noise modeling method based on the Poisson principle. Given a 6D phase-space volume segment including temporal dimension, the arrival of electrons into the volume segment can be naturally assumed to follow Poisson process. Therefore a 6D phase-space volume segment can be represented by a macro-particle sitting at the center[1] of the volume segment whose charge is sampled from Poisson random number of mean weighted by the 6D density of the electron bunch profile. It can be shown that the h-th harmonic bunching factor over a wavelength follows correct statistics if there are enough temporal segments. Explicitly, the h-th harmonic bunching factor b_h is given as

$$b_h = \frac{1}{N_e} \sum_j^M m_j e^{ih\theta_j} \tag{1}$$

where N_e is the electron number in a temporal domain of interest, M is the number of temporal segments or the number of the macro-particles in the domain, m_j is the number of electrons that j-th macro-particle is representing, and θ_j is the j-th macro-particle's FEL temporal coordinate (phase) and is located at the center of the j-th temporal segment. If the domain of interest is one wavelength long, and the number of temporal segments are $2(h+n)$ with $n \geq 0$, then $\sum_j^M e^{ih\theta_j} = 0$. Then, root-mean-square(RMS) bunching statistics become,

$$\begin{aligned} \left\langle b_h b_h^\dagger \right\rangle &= \frac{1}{N_e^2} \sum_j^M \sum_k^M \left\langle m_j m_k \right\rangle e^{ih(\theta_j - \theta_k)} \\ &= \frac{1}{N_e^2} \sum_j^M \left(\left\langle m_j^2 \right\rangle - \left\langle m_j \right\rangle^2 \right) \\ &= 1/N_e \end{aligned} \tag{2}$$

where $\langle f \rangle$ represent ensemble average on f and we used property of Poisson distribution $\left\langle m_j^2 \right\rangle - \left\langle m_j \right\rangle^2 = \left\langle m_j \right\rangle = N_e/M$.

Since the method was derived from the first principle and each macro-particle represent the non-overlapping 6D volume segment, every macro-particle is statistically independent. Therefore, particle migration across the numerical grid can be naturally implemented. Even thoug this method is physically intuitive and clear, it requires a lot of particles to populate the six dimensional phase space.

Coordinate Perturbation and Mirroring

Fawley [3] proposed a shot-noise model that produces correct RMS bunching statistics. The correct initial RMS bunching statistics over $h \leq h_{\max} + 1$ harmonics, where $h_{\max}$ is the maximum harmonic number to simulate, is achieved by the addition of correlated perturbation $\delta\theta_j$ to temporal coordinate (otherwise uniformly distributed such that $\sum_j^M e^{ih\theta_j} = 0$). For example, consider a set of $M = 2(h_{\max}+1)$ particles representing N_e electrons with the temporal perturbation given by

$$\delta\theta_j = \sum_{h'}^M \xi_{h'} \, e^{-ih'\theta_j} \tag{3}$$

* Work supported by the Director of the Office of Science of the US Department of Energy under Contract no. DEAC02-05CH11231

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[1] In original paper [2], there also are small perturbations on 6D coordinates from the center of the corresponding volume. For simplicity, we ignore such perturbation.

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where $\xi_{h'}$ is an instance of a random variable whose statistical property will be discussed soon. Note that the perturbation on a particle is correlated to other particle's perturbation. Then the h-th harmonic bunching factor b_h reads

$$\begin{aligned} b_h &= \frac{1}{M}\sum_j^M e^{ih(\theta_j+\delta\theta_j)} \\ &\simeq \frac{1}{M}\sum_j^M e^{ih\theta_j}\left(1+ih\delta\theta_j\right) \\ &= ih\xi_h \end{aligned} \tag{4}$$

where we used $m_j = N_e/M$. If $\langle\xi_h\rangle = 0$ and $\left\langle \xi_h\xi_h^\dagger\right\rangle = 1/\left(h^2N_e\right)$, then we have correct initial RMS bunching statistics.

$$\left\langle b_h b_h^\dagger\right\rangle = 1/N_e \tag{5}$$

Such a set of particles is called a 'beamlet' in [3]. In order to further model correct evolution of RMS bunching statistics, Fawley mirrored 5D phase-space among particles in a beamlet so that the bunching factor of a beamlet is conserved through drift lines.

It is important to realize that the beamlets are independent of each other while the particles inside one beamlet are not. In addition, note that the temporal coordinates relative to each other among the particles in one beamlet describe microscopic ($\lesssim \lambda_r$, the radiation wavelength) dynamics while the beamlets describe macroscopic ($\gtrsim \lambda_r$) dynamics. From now on, we will call a beamlet by a 'macro-particle' and a particle in a beamlet by a 'micro-particle' so that macro-particles are statistically independent as usual sense.

PARTICLE LOADING AND MIGRATION SCHEME

Here, we present a possible solution pair to the particle migration problem.

Particle Loading

As the 6D volume division requires a lot of particles, we adopt the 5D mirroring strategy among micro-particles of one macro-particle. The main idea of this paper is to interpret one macro-particle to be one statistically independent entity whose temporal coordinate is given by the average temporal coordinate among the micro-particles in it. This way, a macro-particle can be regarded is an instance of the random variable of density probability as usual sense. Once the macro-particles are loaded, each macro-particle is divided into $2(h_{\max}+1)$ micro-particles whose temporal coordinates are uniformly distributed in one wavelength such that the average value is the corresponding macro-particle's coordinate as depicted in Fig. 1. Then add the temporal perturbation following [3] or the charge perturbation following [2] to model physical shot-noise. When charge perturbation is used, one can still consider density variation across the micro-particles' temporal positions and thus can include coherent spontaneous emission [2].

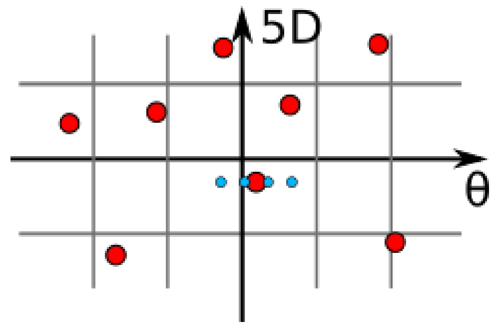

Figure 1: Schematic illustration of macro-particles (red) and micro-particles (blue) consisting a macro-particle.

Macro-Particle Migration Scheme

Since the micro-particles in a macro-particle are not independent of each other, we migrate all micro-particles inside a macro-particle when the corresponding macro-particle migrate across the numerical mesh. The macro-particle migration must be used at least until the numerical shot-noise by the micro-particle migration becomes negligible compared to the FEL interaction induced bunching factor. This macro-particle migration scheme also allows us to use arbitrary weight and shape function for source deposition and field interpolation. Furthermore, it allows using longitudinal mesh size smaller than the radiation wavelength λ_r to increase simulated radiation bandwidth. This is because the weight and shape functions are evaluated at the macro-particle position regardless of individual micro-particles' relative coordinate, and the same value of evaluated weight and shape is shared among the micro-particles inside the corresponding macro-particle. The slippage resolution can also follow the mesh size as one can use moving window unless there is strong coupling between the wiggler period oscillation and the radiation field variation.

Micro-Particle Migration Scheme

As the FEL radiation field develop, the relative 5D phase-space coordinates of the micro-particles start to deviate. This means that the micro-particles start to lose statistical dependence with each other inside the corresponding macro-particle. When the FEL interaction become sufficiently strong, the microscopic dynamics of FEL interaction can influence the macroscopic beam profile. However, if we still use the macro-particle migration scheme, such an effect can not be modeled. More fundamentally, as the micro-particle gain independence from each other, the interpretation of the macro-particle as one statistically independent entity become invalid. Therefore, we need phase transition between macro and micro migration schemes. We observe this transition point using a test example. A more robust criterion to allow micro-particle migration and the method of smooth transition will be studied in the future.

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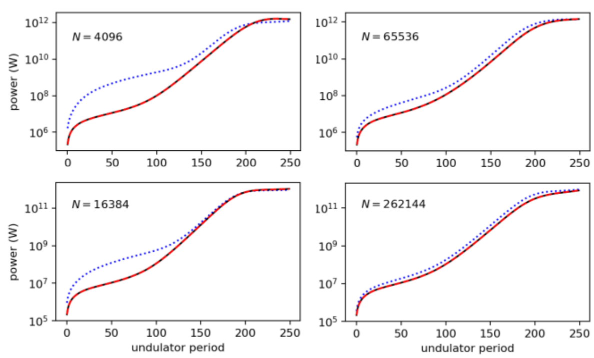

Figure 2: Numerical shot noise by micro-particle migration at SASE start. The black curve is the GENESIS, the red dashed line is when the macro-particle migration scheme is used and the blue dotted line is when micro-particles are allowed to migrate individually. The number of particles used per bunch slice is labeled. 300 slices of electron bunch are used. Each slice corresponds to one numerical mesh of nearest grid point method. The parameters used includes 6D gaussian bunch profile with $\sigma_z = 2\mu\text{m}$, $E = 0.5$ GeV, $\lambda_r = 32$ nm, $\lambda_u = 3$ cm, $I_{peak} = 5$ kA and $K = 1.5$.

ILLUSTRATIVE SIMULATIONS

Here, we present simulation results from two test examples to illustrate effects of the macro-particle and micro-particle migration.

Figure 2 illustrates how micro-particle migration result in unphysical spontaneous radiation and depends on particle number used while the macro-particle migration scheme shows stable agreement with the GENESIS. The parameters are chosen such that the radiation power saturates in a short undulator so that the migration effect is negligible. Note that as the number of particles increases the effect of the numerical shot noise induced by micro-particle migration decreases. The nearly perfect agreement between black (GENESIS) and red dashed (macro migration) is due to good beam quality and short simulation transport that migration hardly happen. The initial particle data was generated by GENESIS and imported into our code. In addition, exactly same mesh number and mesh size are used for both codes.

Figure 2 verifies the need of macro-particle migration. Now, we use enough number of particles so that numerical shot-noise by the micro-particle migration is small. In order to have long enough time to migrate, we used LCLS-II parameters where the saturation length is about 10 times of the Fig. 2. In addition, in order to see the macro-particle migration effect, we introduced energy chirp($\delta_{\text{tail}} - \delta_{\text{head}} = 0.002$). However, Fig. 3 shows nearly zero difference between the GENESIS (no migration) and the macro-particle migration. This is due to nearly identical particle velocities in absence of the dispersive elements like chicanes. Notice that we used large enough number of particles so that there is no initial numerical shot-noise due to micro-particle migration(compare with Fig. 2). Instead, the micro-particle migration starts to show larger and larger difference as FEL interaction develops.

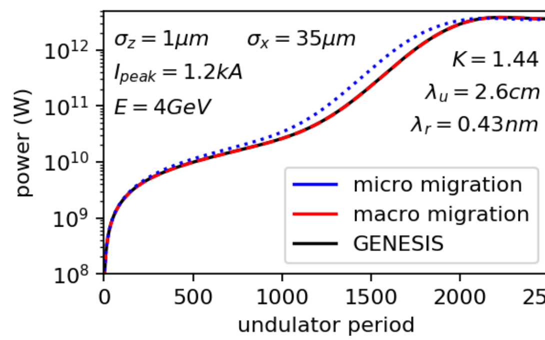

Figure 3: Effect of micro-particle migration as FEL interaction develops. The black curve is the GENESIS, the red dashed line is when the macro-particle migration scheme is used and the blue dotted line is when the micro-particle migration is used. LCLSII like parameters used as shown by texts in the plot.

SUMMARY

A particle migration scheme compatible with 5D phase-space mirroring method [3] of shot-noise modeling is presented. A macro-particle so-called 'beamlet' [3] consists of micro-particles of same 5D phase-space coordinates and different temporal coordinates. A macro-particle is interpreted as one statistically independent entity whose temporal coordinate is given by the average temporal coordinates of micro-particles inside it. Physical shot-noise can be modeled by adding temporal [3] or charge [2] perturbation on each micro-particles. As the micro-particles are not statistically independent, all micro-particles should migrate together when the corresponding macro-particle migrate across numerical mesh until the micro-particles develop independence through FEL interaction. This migration scheme allows the use of arbitrary weight and shape function for source deposition onto mesh points and field interpolation from the mesh points. It also allows us to use temporal mesh size smaller than the radiation wavelength to increase numerical bandwidth. Most importantly, it can greatly reduce the required number of particles to model shot-noise with migration. These are implemented in IMPACT code suite [4].

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